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Electronic and Structural Properties of Si_{10} Cluster

by

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ELECTRONIC AND STRUCTURAL PROPERTIES OF Si_{10} CLUSTER

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Abstract

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I. Introduction

The seminal experimental work at Rice University on small silicon clusters[1] has inspired much theoretical and computational effort to better understand their structure and properties. This has yielded many new results, much of which remain somewhat speculative because the appropriate conditions have yet to be reproduced experimentally. Many researchers have attempted to correlate their computational results with experiment,[2-4] and other workers rely on accurate quantum calculations for their authority.[5-8] Conversely, others have performed imaginative experiments so as to shed some light on the theoretical problem.[9-11]

Most recently, two techniques have emerged which seem to set the issue of structure largely to rest. Both are based on molecular dynamics methods to allow the structure to arrive at an equilibrium position. The first of these, ab initio molecular dynamics,[12] indicates two structures nearly degenerate in energy: a distorted, tetracapped triangular prism (TTP) and a tetracapped octahedron (TO) (see Fig. 1). More recently, Chelikowski et al[4,13] have used a classical potential (thermodynamic force field) method, yielding the bicapped tetragonal antiprism (BTA) as the most stable structure. These results are in general agreement with the ab initio total energies of Raghavachari and Rolfing[6,7] for various structures. However, there is not, as yet, a conclusive determination of the minimum energy structure of Si_{10}, and none of the published HOMO-LUMO "band gaps" fit the experimental data, nor is there a satisfactory explanation of the reactivity data.[9] Furthermore, the effects of charging the cluster are not known.

In this article, we use the tight-binding (TB) method to calculate the cohesion energies of all structures of the Si_{10} cluster listed above. We also consider the positive and negative ions. Our work yields results very close

to those of Refs. 7 and 13, except that we find Jahn-Teller effects to be very important. We conclude that the most stable form is a distorted BTA (DBTA) structure with C_2 symmetry. Most importantly, we are able to fit our results with both the photoelectron spectroscopy (PES)[11] and the reactivity experiments.[9]

We are interested in the extent to which the TB model yields information about the excited states. In particular, we aim at evaluating the "band gap" of the clusters and examine the possibility of obtaining transition matrix elements for the first electronic transitions. It is known that the local density approximation (LDA) band structure underestimates the band gap for solids and large systems, and high-accuracy ab initio methods cannot deal with large systems. A semiempirical TB method, which is parametrized to fit the band structure of the bulk, on the one hand, and matches the binding properties of the dimer, on the other hand, circumvents these problems. The TB parameters are chosen to correctly model the band gap in the solid,[14] and they model the direct band gap quite accurately. They also give a reasonable approximation of the indirect band gap.

The goal of this work is to demonstrate that the model can be extended to the electronic structure of clusters as well. This will allow us to calculate the optical properties of silicon clusters, especially as a function of structure and/or surroundings. Therefore, we show that the HOMO-LUMO gap for our most stable structure is consistent with experiment, and thus we contend that the TB model is accurate in this regard, at least for one-electron levels near the Fermi level. For application to clusters, however, the bond definition and the total number of bonds is a parameter in the TB model. We investigate the bond number dependence under circumstances in which "partial bonding" may occur.

We have chosen Si_{10} as our model system, since it is the cluster for which the maximum amount of data are available, both experimental[1,9,11] and computational.[5-7,12,13,15-18] We find that the TB model reproduces the previous calculations qualitatively, and the quantitative differences can be accounted for. Further, the simplicity of the calculation allows us to try a diverse group of isomers and ions. Our interest in the electronic properties may provide an experimental handle with which to finally resolve the geometry question.

The next section briefly describes the method used in the calculation. Section III then contains the results of the calculation, and Section IV offers a brief conclusion.

II. Method

The tight-binding model is used as described in several previous papers.[2,3,14-16] The parametrization for silicon, developed by Chadi[14] for the study of surfaces, was modified by Tománek and Schlüter to reproduce ab initio results for the dimer.[15,16] This results in a classical repulsion energy, which is then added to the attractive TB energy. In addition, it is necessary to account for varying coordination numbers. In the bulk, the coordination number is always four, but in smaller clusters, the number of nearest neighbors ranges from one to eight. Hence a term which depends on the number of bonds in the cluster was also added.[16] Thus the method is really a mixed breed, quantum insofar as the bulk properties are concerned, and "classical" with respect to the repulsive interactions.

From the electronic structure it is possible to obtain the transition matrix elements. As a test of the method, we will calculate the static polarizabilities of different clusters. Through a Mulliken population analysis, the TB model yields the charge density distribution among atomic

sites within the cluster. From this, the transition dipole matrix elements can be approximated as

$$(r_i)_{ng} = \sum_{\mu} R_{\mu i} \sum_{p} c^{*}_{n\mu p} c_{g\mu p} \quad , \qquad (1)$$

where $r_i = (x, y, z)$, $R_{\mu i}$ are the corresponding coordinates of the nuclei at sites μ, and g and n refer to the ground state and excited one-electron states c. This is a reasonable approximation only for a large molecule or cluster, where the valence charge is sampled at the atomic sites, of which there are a sufficiently large number. However, this procedure should be an improvement over the bond-charge model[19] and charge-transfer model,[20] which have been successfully used to evaluate the nonlinear optical properties of solids.[21]

The total energy and electronic structures obtained depend on the total number of bonds in the cluster. In our model, two atoms are considered bonded when the interatomic distance is less than the cutoff value, for which we have used 3.30 Å. This is the distance which is approximately between the nearest neighbor and next-nearest neighbor in the bulk, and it yields results which are consistent with those of Tománek and Schlüter.[16] Except in one special case, described below, varying this parameter has no effect on the result.

We find that the one-electron levels are very sensitive to the geometry, and that very minute changes in the structure wreak large changes in the energy levels. For this reason, the minimization of the total energy through geometry optimization is crucial. Thus we first use Hellmann-Feynmann forces to come close to equilibrium, and then a multivariable minimization technique to optimize the structure without symmetry restrictions.

IV. Results

The TB model has been used to evaluate the structure and electronic properties of four isomers of Si_{10}. These are TTP, BTA, TO and A, as illustrated in Fig. 1. There exist at least two stable forms of distorted BTA (DBTA-I and DBTA-II). The DBTA-I structure differs from BTA in that it is stretched in one dimension and squeezed in another, and hence there is an additional bond (or partial bond) with a length of about 3.30 Å, as illustrated in Fig. 2. This reduces the symmetry of the species from D_{4d} to C_2. DBTA-II contains no additional bonds, but involves a stretching and twisting of the original BTA form, also with C_2 symmetry. All BTA-related structures are stable in that there is a local energy minimum for that configuration, but obviously the activation energy between them is very low.

Chelikowski et al[13] report the BTA structure as being most stable, whereas Andreoni et al[12] cite TTP as the energy minimum. Reference 6 gives TO as the most stable structure, while Ref. 7 suggests that TTP is slightly more stable. Raghavachari and Rolfing[7] have investigated BTA in two different electronic configurations; however, their method of calculation does not include the geometric effects of distortion. Within the accuracy of our calculation, the BTA and TTP forms appear to be degenerate, but neither matches the PES experimental data. There is no band gap for BTA, and for the TTP the HOMO-LUMO transition is 2.6 eV. The latter value is consistent with that reported for the same structure in Ref. 12. The experimental value observed by Cheshnovski et al[11] is 1.2 eV.

Given the degeneracy of the Fermi level for BTA, it is not unreasonable to suppose that Jahn-Teller effects are important. Indeed, careful optimization of the geometry reveals two structures which are related to BTA, but less symmetric. The most stable, DBTA-I, actually involves an additional

partial bond, and thus has a different topology than BTA. It could, therefore, be considered a different structure entirely. Nevertheless, it has C_2 rather than D_{4d} symmetry, which breaks the Fermi-level degeneracy. As shown in Table I, this turns out to be the most stable configuration. Further, the HOMO-LUMO transition is calculated as 1.4 eV with the 25th bond, and 0.9 eV without it, which matches the experimental result closely. This is the bond number effect, from which we conclude that there is probably a partial bond replacing the one in question. Nevertheless, a comparison of both the HOMO-LUMO gap and the energies indicates that retaining the bond fits the experiment more accurately. The coordinates of the DBTA-I structure are given in Table II.

The bond dependence of the model also shows up in the results for TO. In this case, the TB results may yield too low a cohesion energy, since the repulsion energy may be over estimated, being calculated independently of the coordination number. The TO form contains six hexa-coordinated atoms, more than any other form. This effect can be seen by considering the calculated bond lengths for TO. In our calculation (and also in Ref. 16), the bond length between atoms in the octahedron (hexa-coordinated) is 3.0 Å, compared with 2.5 Å as the ab initio result. Conversely, the bonds connecting the cap atoms (tetra-coordinated) are about 2.4 Å in both methods. The cap atoms have the lowest coordination numbers, and it is seen that the TB model reproduces the other results more accurately in this case. However, while the TB energy may be inaccurate, it remains true that the TO data does not fit the PES spectrum for any of the above calculations, and thus has to be excluded as a plausible structure.

The adamantane structure is a 10-atom fragment of the bulk solid, and is an open rather than a close packed geometry. As a result, it only has an

average coordination number of 2.4, only half that of the other structures. Our calculation agrees with the results of Ref. 16 in that we find the form to be unstable. Geometric optimization rapidly leads to the formation of additional bonds.

It is interesting to note that, with the exception of DBTA-I, all stable structures contain 24 bonds, with an average coordination number of 4.8. This compares with a bulk value of four. Since the number of bonds does depend on the cutoff value, we have illustrated the bond lengths and other interatomic distances in Fig. 3. It is seen that, with the exception of DBTA-I, varying the cutoff value between 3.05 and 3.55 Å will not change the result. Thus we conclude that our results are largely independent of the precise value of the cutoff distance.

The above conclusions also explain the reactivity results nicely.[9] Given the probable low activation energy between the BTA-related forms, it should be useful to lump them together as one species. We have estimated the electron affinity of each isomer by listing the energy of the LUMO level in Table I. This is an indication of the propensity of the isomer to accept an additional electron, i.e., the lower the LUMO level is, the greater is the electron affinity. Indeed, our LUMO state differs from the electron affinity primarily because our zero-point energy is taken as the HOMO level in the bulk, rather than the energy of an electron removed to infinity. Similarly, a small HOMO-LUMO gap indicates a greater reactivity, since this implies that valence electrons have a greater freedom to rearrange in bond formation. It can be seen from Table I that the BTA-related structures have a greater electron affinity and a smaller band gap, implying that they are relatively reactive. Conversely, TTP has a low electron affinity, indicating low reactivity. Thus the reactivity results of Ref. 9 can be explained, where it

has been concluded that two isomers of Si_{10} exist, with the most common (85% abundance) being approximately an order of magnitude more reactive than the other. If BTA-related forms constitute the abundant isomer, with TTP being the minority, then the electron affinity results just presented conform with the experimental data. Further, the energy difference approximately describes the Boltzmann distribution between the two forms at room temperature.

While calculations for ionic species must be considered less reliable, the data for the anion species confirms the above hypothesis. In the anion case, it is found that DBTA-I is unstable, and that it reverts to the DBTA-II anion, which is more stable that the neutral species. It can thus be seen that the electron affinity for DBTA-I is probably greater than is indicated by looking at the LUMO level. The DBTA-II structure is closer to BTA, and so the Jahn-Teller effect is smaller. This is consistent with a model in which the additional electron affects the degeneracy of the BTA structure. Accordingly, we hypothesize that the doubly-ionized cluster would be stable in the BTA form.

Having thus established the TB method as reliably reproducing experimental data, we now wish to calculate the static polarizabilities for the various clusters. Using Eq. (1) for the dipole matrix elements, we have evaluated the perturbation expansion[21] for the static polarizability α of the clusters. We obtain a value of about 1×10^{-22} esu for all of the structures. An improved calculation to be outlined in a subsequent paper yields approximately 1.4×10^{-22} esu. This result is generally independent of the band gap, and it depends on contributions from several transitions (not only near the HOMO-LUMO transition). The three components of α for TTP and TO are almost equal, reflecting the approximate spherical symmetry of these species, whereas α_{zz} for DBTA is stronger, given the spatial extension in that

direction. The polarizability should assume a value generally equal to the size of the molecule, which in our case implies an atomic diameter of approximately 2.6 Å. As can be seen from Fig. 3, this is a reasonable value. Thus we conclude that the TB model not only correctly predicts the structure of the species, but also yields information about the optical properties, at least qualitatively.

IV. Conclusions

In summary, it can be concluded that the TB model generally yields reliable results for the structure of small silicon clusters. This is confirmed by our present study of Si_{10}, and previously established[16,17] for smaller clusters through comparison with ab initio Hartree-Fock[6,7] and LDA[16] calculations. Further, in this paper we have shown that the TB method provides information about the electronic structure sufficient to account for experimental PES and reactivity data. The parametrized, semiempirical nature of the model allows for a simple calculation with little cost in accuracy. More sophisticated quantum techniques, while expected to be as (or more) accurate, and certainly more fundamental, are also much more lengthy and thus less flexible.

We have found that a distorted form of the bicapped tetragonal antiprism is the most stable structure for the Si_{10} cluster. In addition, the HOMO-LUMO "band gap" and electron affinity data correspond with experiment. We view this as a justification of our original hypothesis, namely that the TB model, optimized for a solid, can be used for clusters, and can yield some information about excited states. Our results are consistent with previous work, most notably Ref. 13, in which BTA is proposed as the stable configuration. Since that calculation was done using a classical force field,

Jahn-Teller effects would not show up, and so distortions from symmetry would not be readily apparent.

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TABLE I

Species	Cohesion Energy (eV/atom)	HOMO-LUMO Gap (eV)	LUMO Level (eV)
DBTA-I*	-3.98 (-3.92)	1.4 (0.9)	+0.18 (+0.13)
DBTA-II	-3.92	0.6	-0.50
BTA	-3.90	0.0	-0.92**
TTP	-3.91	2.6	+1.21
TO	-3.61	2.9	+2.00

* The values for the 24-bond structure are given in parentheses.

** Since the ground state is degenerate, this is also the HOMO level.

Table I. Cohesion energies, HOMO-LUMO transition energies and LUMO energies of various Si_{10} structures, shown in Fig. 1. The LUMO one-electron energy, which is a rough indication of the electron affinity, is given relative to the "HOMO" level of the bulk.

TABLE II

Atom #	X (Å)	Y (Å)	Z (Å)
1	-1.33	-1.42	1.10
2	-1.33	1.42	1.10
3	1.33	1.42	1.11
4	1.33	-1.42	1.11
5	-1.61	0.00	-1.07
6	1.61	0.00	-1.07
7	0.00	-2.11	-1.04
8	0.00	2.11	-1.04
9	0.00	0.00	2.73
10	0.00	0.00	-2.92

Table II. Atomic coordinates of the 25-bond version of DBTA-I. The 24-bond version differs only in the second decimal place.

FIGURE CAPTIONS

Fig. 1 Structures for BTA (a), TTP (b) and TO (c). Adamantane is not shown. Distances are in Å.

Fig. 2 Structures for DBTA-I (a) and DBTA-II (b) clusters, with distances in Å. In DBTA-I the additional bond is shown by a dashed line.

Fig. 3 Range of bond lengths for different isomers. The cutoff parameter chosen (3.3 Å) is shown by the dashed line. The thick bars below illustrate the range of bond lengths in the cluster. The thin bars above indicate the range of non-bonded distances, with the upper limit corresponding to the maximum diameter of the cluster. For DBTA-I two possibilities are indicated. On the left, the 25-bond form is shown, whereas on the right, the 24-bond form is shown.

Fig. 1 (a)

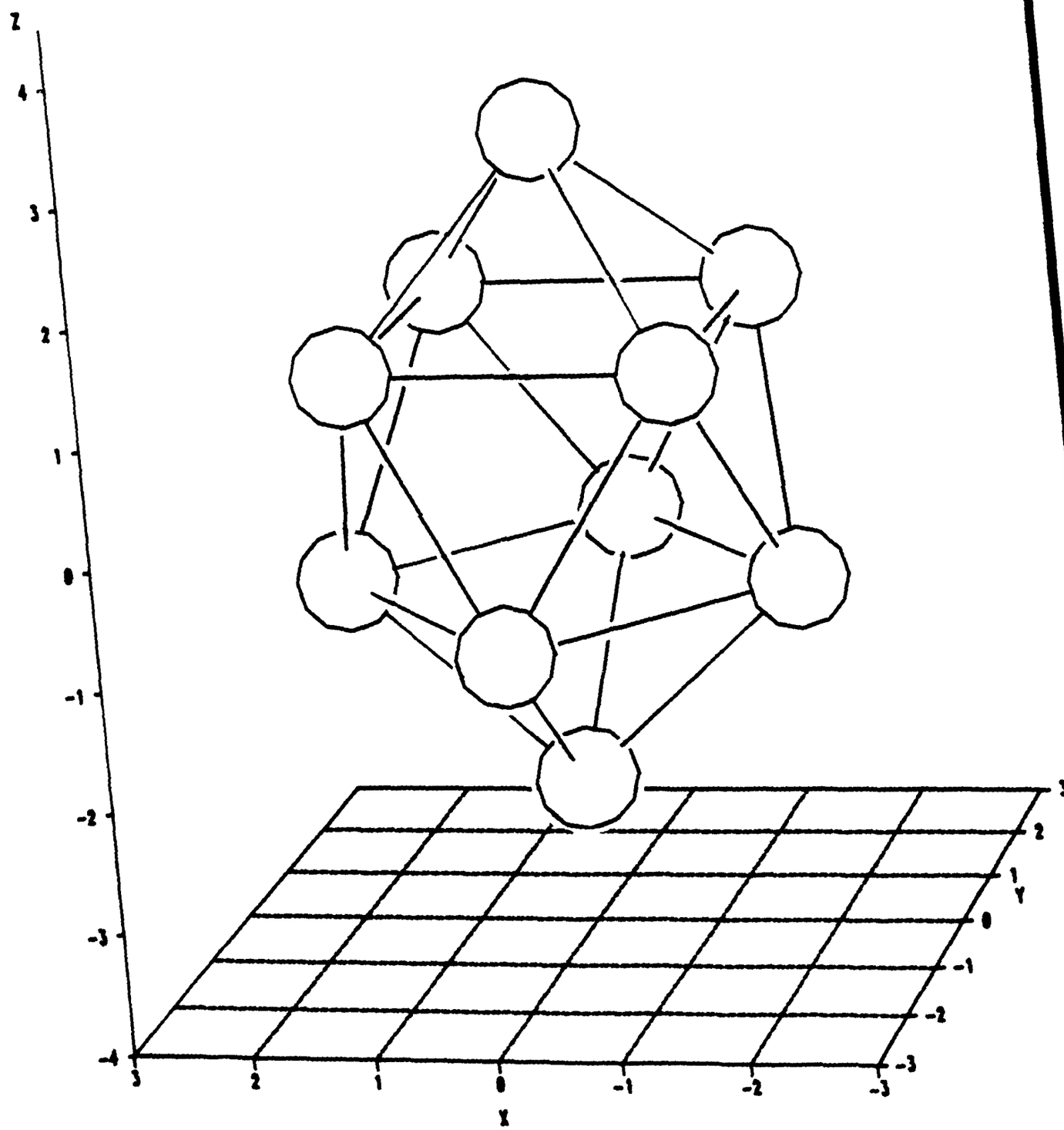


Fig. 1(2)

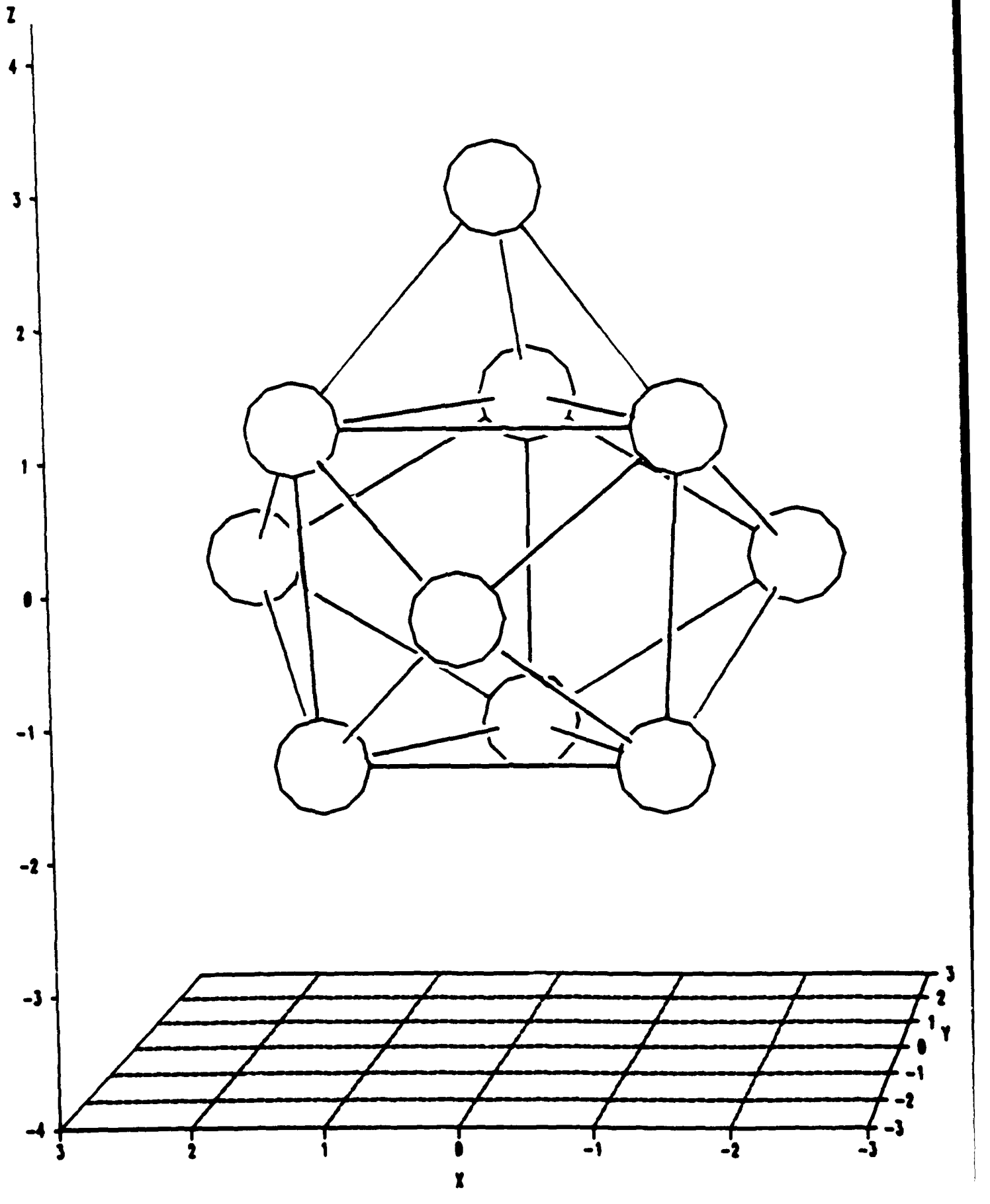


Fig. 1(c)

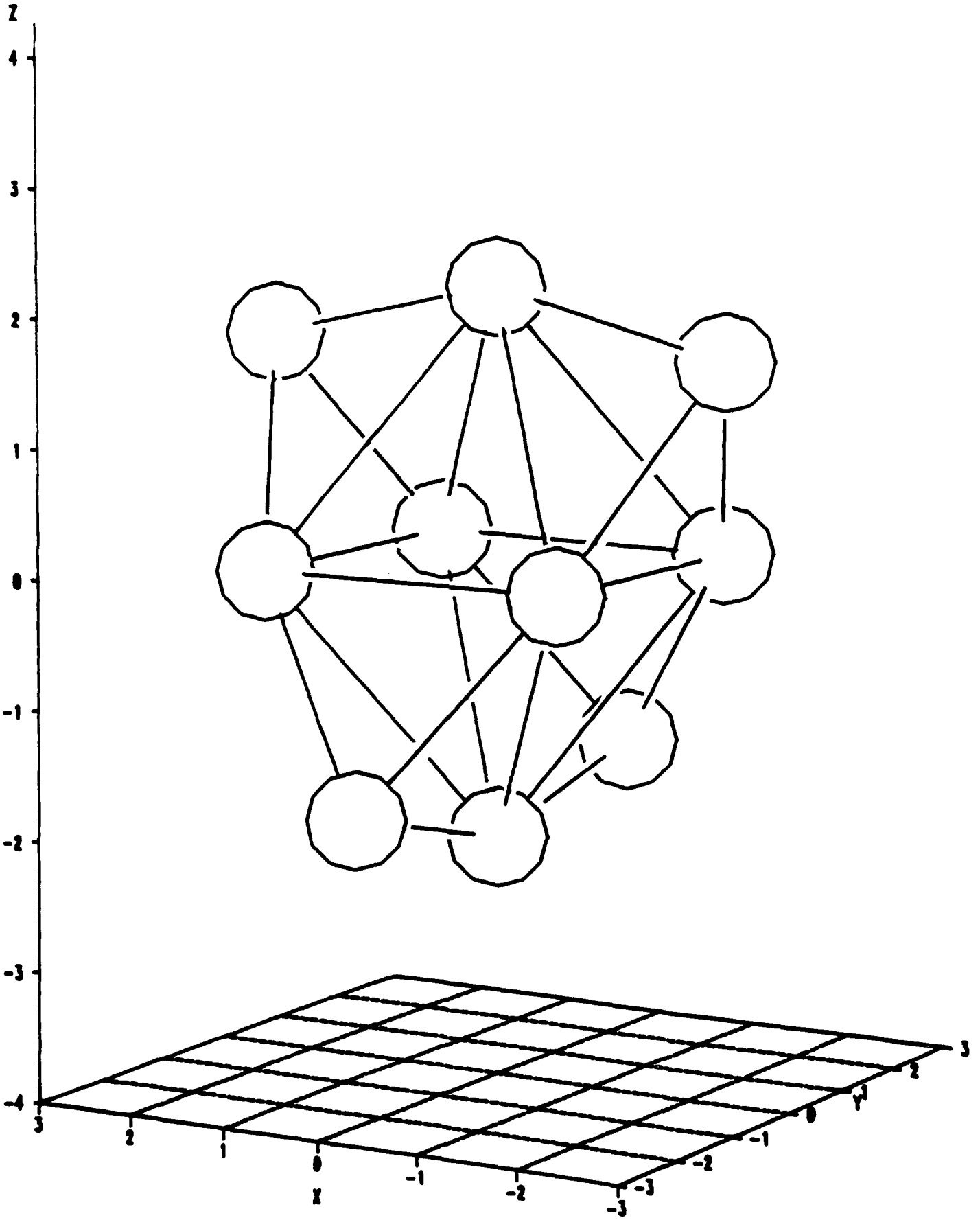


Fig. 2(a)

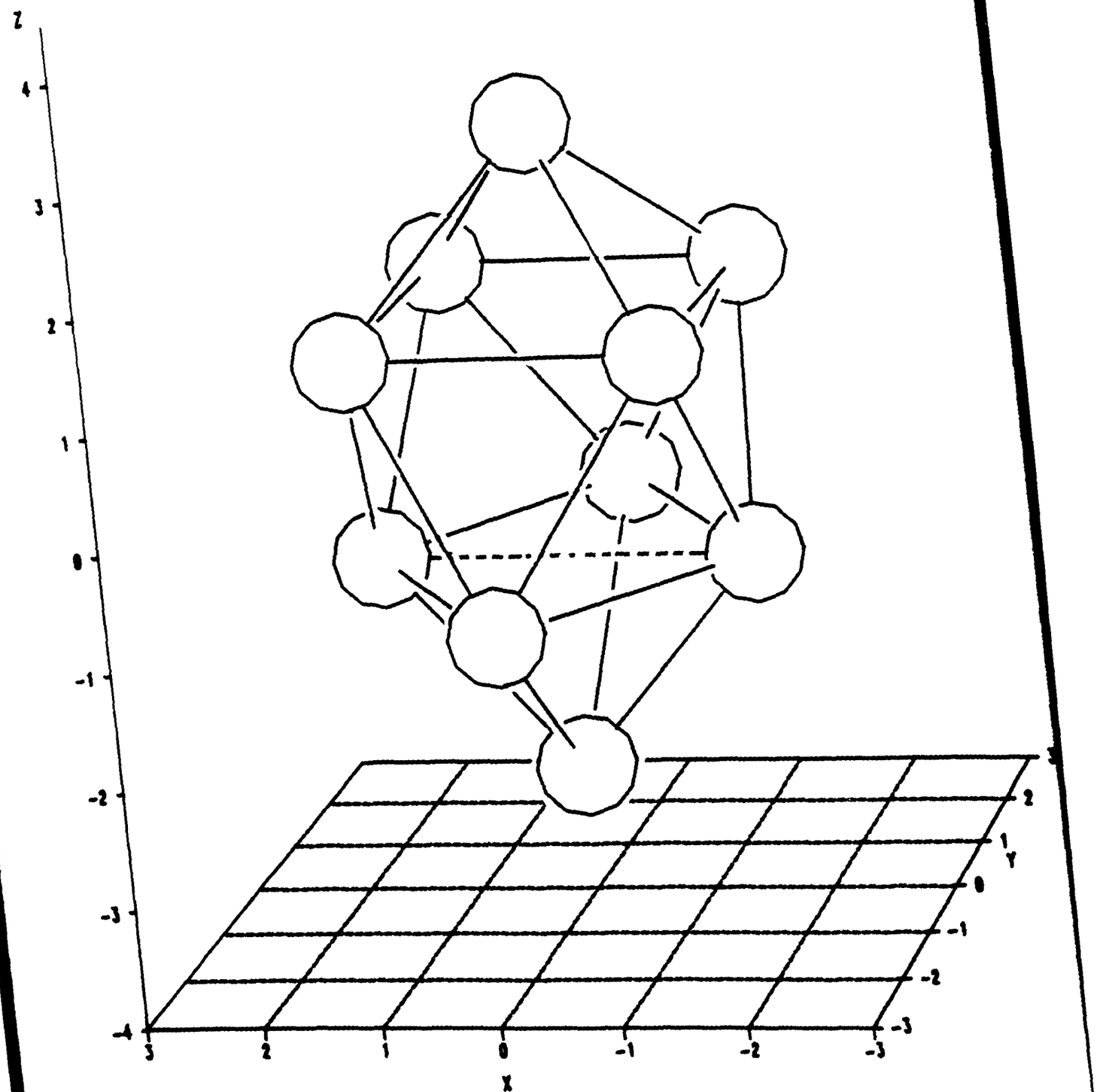


Fig. 2(b)

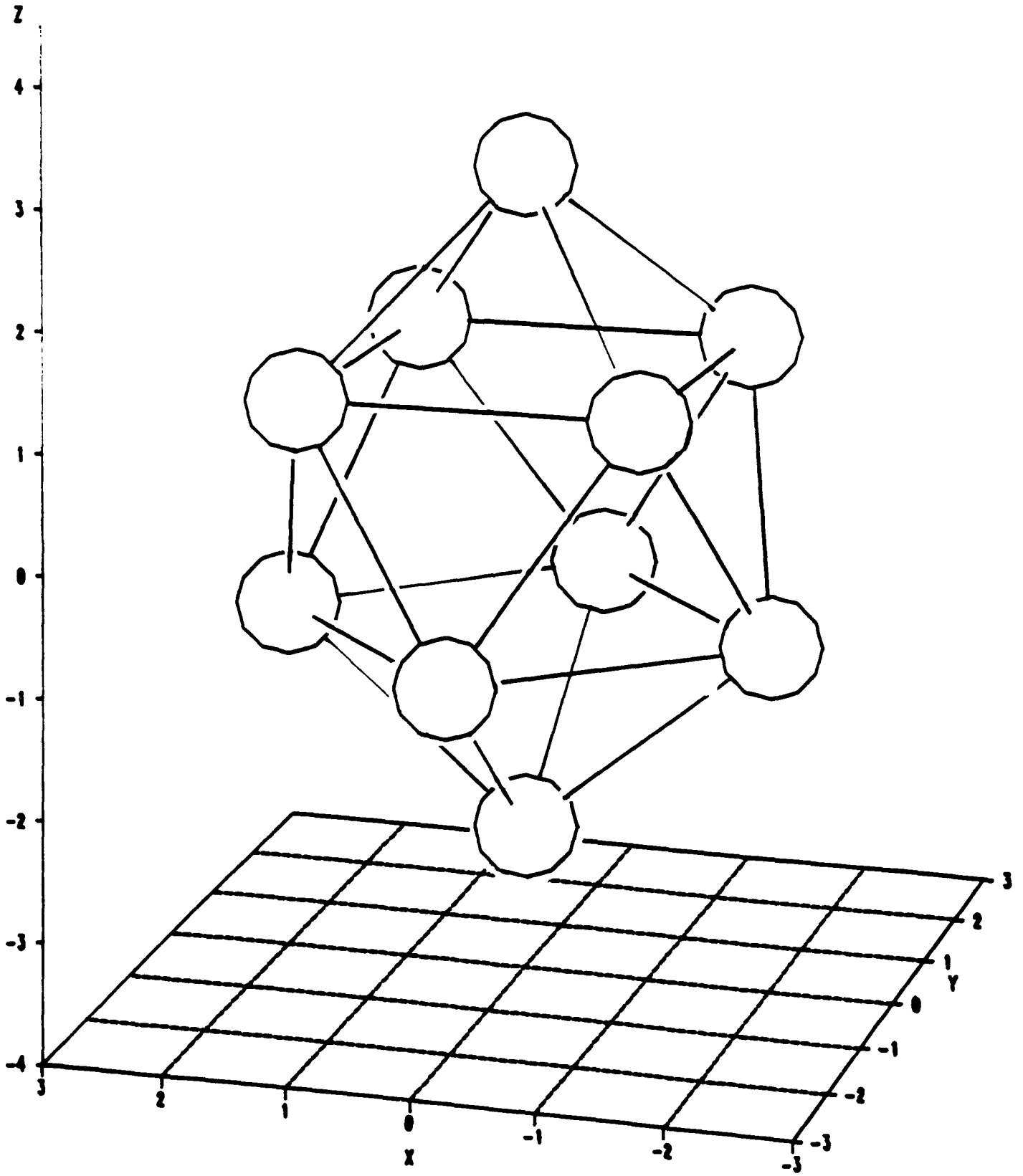
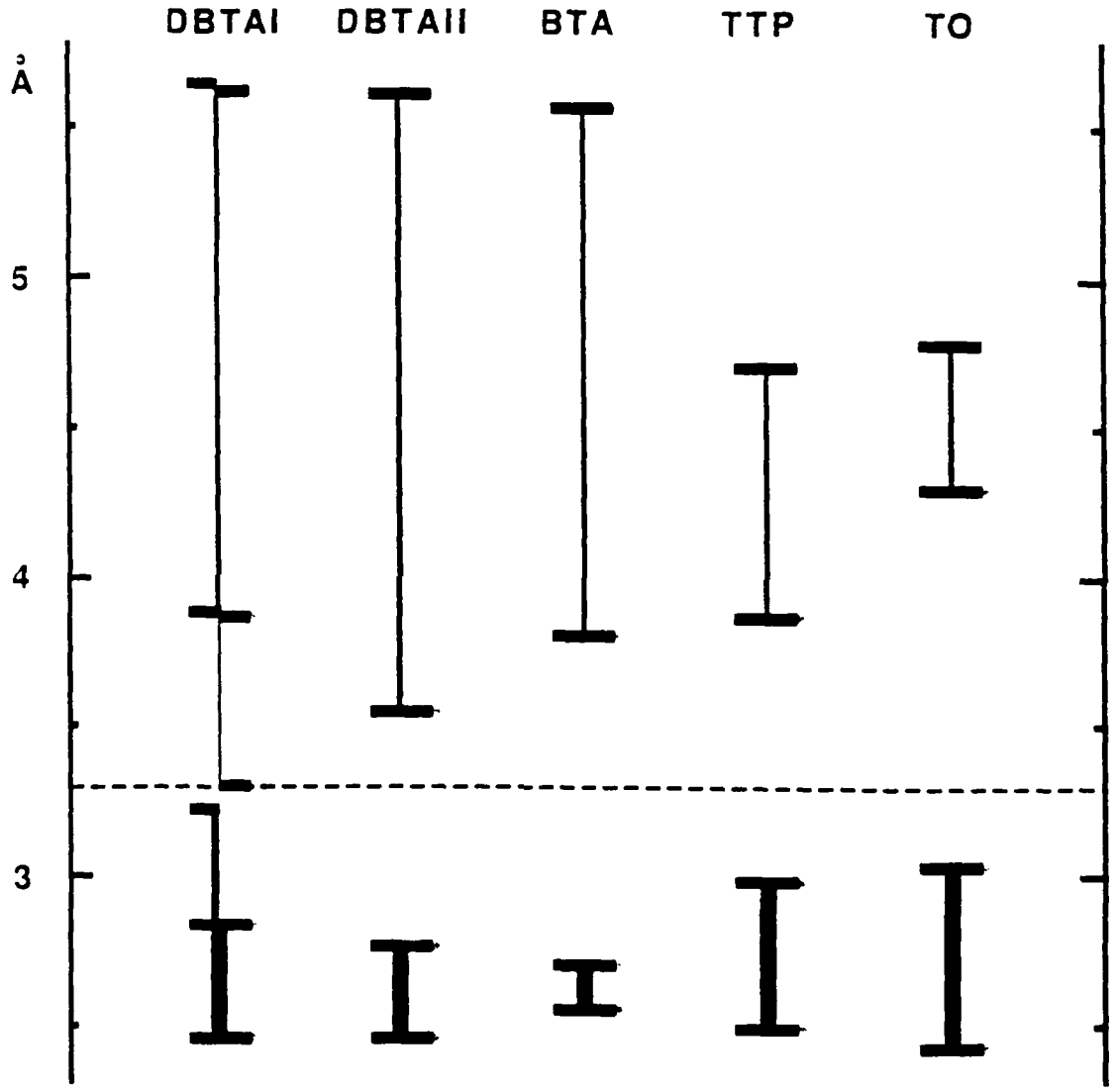


Fig. 3



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